

**Table S4.** List of most important coordinates for weight vector learned by linear SVM using all high-confidence experimental data. Zif268 ‘classical’ contacts are highlighted.

position	amino acid	base	weight
2	H	g	4.611
3	R	g	4.443
3	I	t	3.434
4	S	g	3.425
4	V	c	3.011
3	L	t	2.595
3	S	t	2.469
2	H	a	2.387
2	K	g	2.215
3	H	t	2.212
3	S	c	2.202
3	G	c	2.075
1	S	c	2.049
2	A	t	2.014
2	S	t	1.995
2	D	c	1.904
3	W	t	1.779
2	N	a	1.731
1	R	g	1.588
2	Q	c	1.525
3	Q	a	1.51
3	N	t	1.142
3	T	t	1.14
4	Q	a	1.12
4	S	a	1.099
2	Q	a	1.086
4	T	a	1.075
4	C	g	1.071
4	M	c	1.035
1	L	g	0.896
4	H	c	0.758
1	Q	c	0.653
2	L	c	0.653
1	T	t	0.644
1	N	c	0.567
1	V	a	0.554
3	Y	g	0.537
4	Q	c	0.528
4	R	g	0.489
1	H	t	0.485